Fast Adaptive Multiresolution Analysis and Low-Separation Rank Approximations of Functions in High Dimensions

George Fann*, Gregory Beylkin† and Robert Harrison‡

We derive and investigate adaptive analysis-based scalable methods for nonlinear approximation of multi-variable functions which may have singularities or discontinuities in the spatial or Fourier domains. These approximations are used to derive fast methods for application of free space and quasi-periodic Helmholtz Greens functions. They are also used to develop high-order methods for solving time-dependent multiparticle Schrdingers or scattering equations. These equations (6-D and 9-D integro-PDEs) are derived from models in computational chemistry, material science and nuclear physics. In addition, we develop an algorithm for inverting a bandlimited Fourier Transform that avoids both the use of windows and the Gibbs phenomenon. This algorithm is based on constructing approximations of functions via short sums of exponentials. Initial implementations are realized in the software package MADNESS.

*Computational Mathematics Group, Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830. This research is sponsored by the Office of Advanced Scientific Computing Research; U.S. Department of Energy. The work was performed at the Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC under Contract No. De-AC05-00OR22725.

†Department of Applied Mathematics, University of Colorado, Boulder. CO. This research is partially supported by DOE/ORNL grant 4000038129, DOE grant DE-FG02-03ER25583.

‡ORNL/UT Joint Faculty, Computational Chemical Sciences Group, Computer Science and Mathematics Division, Oak Ridge National Laboratory, and Department of Chemistry, University of Tennessee, Knoxville. This research is partially supported by the Office of Basic Energy Sciences; U.S. Department of Energy. The work was performed at the Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC under Contract No. De-AC05-00OR22725.